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BEYOND MERE AUTOMATION

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Abstract - The advent of microprocessors has extended the advantages of automation to every level of instrumentation. Now microprocessors are opening the way to intelligent instrumentation--beyond mere automation. These are instruments that test and calibrate themselves, optimize their operation, and become part of a network of distributed intelligence. Examples in our laboratory include the intelligent management of a linear diode array detector, a multiple microprocessor system for simultaneous execution of related tasks in a triple quadrupole mass spectrometer, and a hierarchical system of minicomputers and single and multiple microcomputers. Microprocessors can handle many variables, adapt to a large variety of transducers, control operations at high speed and perform complex data interpretation. These capabilities will soon have a profound effect on chemical instrumentation, not only in automation and intelligent control, but in new basic design concepts and dramatically enhanced measurement capabilities. Some likely directions for future developments are explored.

INTRODUCTION

Modern chemical instruments are performing feats in our laboratories every day that would have seemed incredible only a decade ago. Sensitivities in parts per billion and selectivities that provide direct analyses for samples with hundreds of components are examples of capabilities that have had far-reaching consequences in both science and society. Are we approaching a plateau in this most-recent advance in scientific measurement capability or are there still more dramatic developments just around the corner? My own opinion is that we are just at the beginning of an exciting new era. I will try to develop the bases for this conviction during this talk.

When we let our imaginations go, the possibilities of total analysis systems for serum, urine, crude oil, or river water do not seem very far fetched. Serious work is going into systems for the automatic amino acid sequencing of micro amounts of proteins. Perhaps even the fictional "Star Trek" analyzer, which not only performs a total analysis on whatever it is aimed at, but only reports those results relevant to the immediate problem, is not completely absurd. Such instruments can dynamically alter the analytical procedure to fit varying conditions and are intimately involved in the interpretation of the results. As such, they are well beyond mere automation. Until recently, we would have considered these possibilities pipe dreams, but today, we have almost become accustomed to the technologically incredible--and the principal cause of this revolutionary expectation is the microprocessor--the so-called "computer on a chip."

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MICROPROCESSORS IN INSTRUMENTATION

Actually, the *microprocessor* is just part of a computer on a chip (or on a few chips). The complete computer as shown in Fig. 1, consists of the central processing unit (CPU), some memory, and enough peripheral devices for it to function as a *microcomputer* (1). The microprocessor integrated circuit (IC or "chip") itself includes at least the CPU, but can also include modest amounts of memory, some device interfaces, and timers. The microprocessor, by itself is a sequencer, a communicator, and a processor. That is, it will

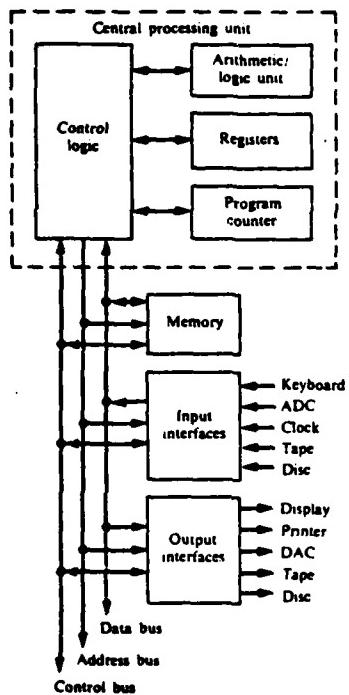


Fig. 1 Taken from reference (1) with permission.

follow a prescribed sequence of instructions (a program), it will transfer data between devices, memory, and its own registers along the bus, and it can perform logic and arithmetic operations on data in its registers. As we shall see, ways to input and output data are required for the microprocessor to act as a *microcomputer*.

Beside doing the usual computational sorts of things, microprocessors can also be involved in both measurement and control operations in instruments. Signals from analog transducers can be applied to an analog-to-digital converter (ADC) and transferred along the bus for storage and/or processing. Similarly, data representing control quantities can be transferred to output ports to effect changes in the instrument operating conditions. If the controlled device, such as a heater, is combined with a temperature-measuring input, the microprocessor can operate as the dynamic element in a feedback system for temperature control. Since the microprocessor may only have to spend a millisecond or so every few seconds in the control program to maintain the desired temperature, it would have plenty of time to perform other functions as well.

Historically first, and still important, is the *computer-controlled instrument*. A block diagram of this class of instruments is shown in Fig. 2.

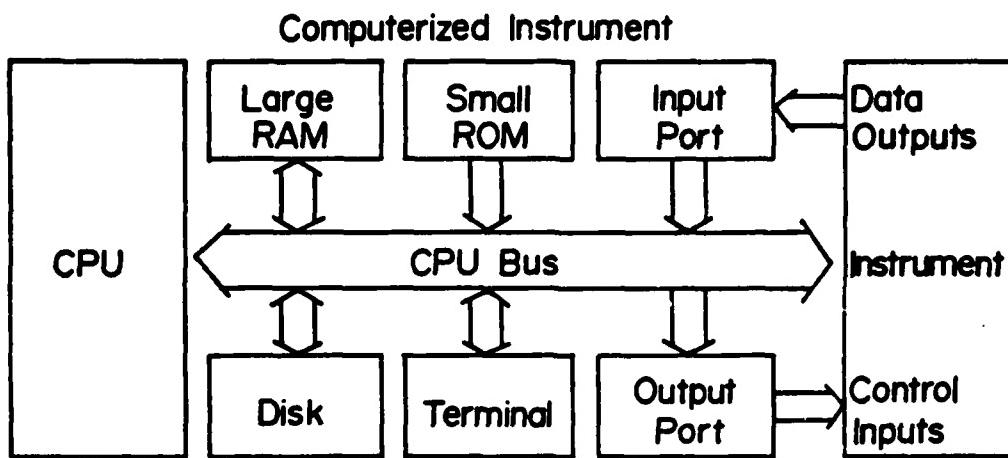


Fig. 2 Computerized instrument

- Needs: a) Disk or tape for program storage and loading.
- b) Operating system for program development, loading, and execution.
- c) Programming language(s)

The computer part is in its traditional format with a disk to load programs and an operating system. The operator runs the computer and through it, the instrument. Independent instruments have become "computerized" in this way by being interfaced to one of the several available forms of "laboratory" computers. Many of the larger commercial computerized instruments such as X-ray spectrometers and mass spectrometers follow this same format. The operator must become proficient with both the computer and the instrument operations. In the extreme case, the entire instrument--all its adjustments and settings--would be under computer control. Every operation could be automated and all control would be through the terminal.

Another implementation of the microprocessor in instrumentation is as a *process controller* as shown in Fig. 3. The CPU in a process controller is not set up to operate as a general

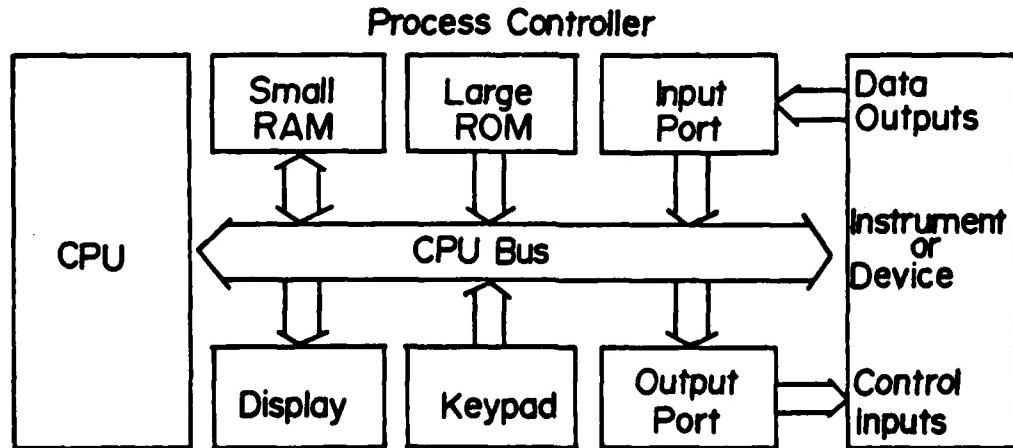


Fig. 3 Process controller

- Needs: a) Programs for all needed functions in ROM
- b) Way to generate ROM-based programs

purpose computer, but rather as a limited function controller (2). The programs for the desired instrument functions are contained in permanent read-only-memory (ROM) so that no operating programs need to be loaded. Little or no provision is made for program revision or addition, so no operating system or compiler programs are required. The keypad control panel and the display can be greatly simplified by indicating directly the limited number of commands and messages that will be used. The hand-held calculator and computer games are examples of limited function process controllers; so are microprocessor-controlled pH meters, spectrophotometers, digital integrators, etc.

INTELLIGENT INSTRUMENTS

The versatility of the microprocessor as a sequencer is very great. Besides following a list of commands in order, it can also follow a loop of commands or branch to a new set of commands depending on the results of its many possible operations. Thus procedures can be altered depending on the outcome of tests or measurements. In this way the microprocessor can implement or reflect the intelligence of its programmer in a dynamic way during the functioning of the instrument. Its ability to make and carry out such decisions on a microsecond time scale allow computer-based instruments to not only eliminate tedious operations, but to implement human intelligence in operations and processes that are beyond human capability.

TABLE 1. Examples of intelligence in instruments

1. Won't execute an inappropriate command
2. Responds to high-level commands
3. Aids operator in effective instrument use
4. Aids operator in interpreting data
5. Calibrates itself automatically
6. Tests its own operation and diagnoses failure
7. Dynamically optimizes data collection

Table 1 gives some examples of functions or characteristics that might be found in intelligent instruments. In each case, decisions or interpretations are made by the computer that make it appear to have some sense, rather than just blindly following a predetermined sequence no matter what. Since the degree of intelligence in an instrument (after it is completely interfaced) depends only on the sophistication of the program and the availability of computer time to execute it, more and more of these intelligent functions are appearing in computer-based instruments. There are programs that help the operator select and load the appropriate data disk and there are programs that match spectra or retention times with library data, label the data display, and write a report. Self-calibration and self-diagnosis can greatly enhance reliability and reduce the skill level required of the operator.

In the May, 1981 issue of Analytical Chemistry, Bruce Kowalski reported a possibly prophetic conversation he had with his somewhat smart alec computer (3). It reminds him that if he asks for the complete results of a particular analysis it will take him two hours to read it and it suggests they (!) publish the successful results of the implementation of a new computational algorithm the computer decided to try.

No matter how bright the computerized instrument, however, it cannot tell you more about the sample than is in the data it has collected. Advances in the analytical power of instrumentation can then proceed along two tracks: One is that of the chemometrician who wants to make sure that all of the real information possible is extracted from the data available. The other is that of the instrumentalist who explores the possibilities of designing instruments that can provide more useful data. Both approaches are valuable and both depend, in their way, on the intimate involvement of the microprocessor.

NEW DIMENSIONS FOR INCREASED CHEMICAL CAPABILITY

The analytical power of an instrument is increased if, without degradation of other characteristics, one can increase sensitivity, selectivity, or throughput or decrease the required sample work-up or cost. These factors are all interrelated in different ways for different techniques, but for most techniques, the sensitivity is not limited by the ability to detect smaller amounts of the analyte, but rather by the presence of other sample components that affect the instrument's response. This is a kind of "chemical noise" that is most often reduced by invoking additional refinements in the chemical work-up--often at the expense of cost and throughput. The amount of chemical noise present

in a technique is inversely related to its selectivity. In other words, the more specific the technique is for the monitored species, the less work-up is required and the more sensitive it can be for real-world samples.

The immense success of gas chromatography/mass spectrometry (GC/MS) is due to the combination of the high selectivity of GC with the highly characteristic identification provided by MS. With its associated computer, called a data system in this case, the GC/MS instrument records mass spectra at regular increments of elution time throughout the GC run. The complete experimental data is then sometimes plotted to show its three dimensions--mass and time along the two axes in the horizontal plane and ion intensity as a contour above that plane. Clearly the three-dimensional contour contains very much more information about the sample than exists in either the chromatogram or the mass spectrum.

A number of other multidimensional instruments have also been developed recently. One example is excitation/emission fluorescence. Fig. 4 is a data plot obtained by Hershberger, Callis, and Christian (4) from an instrument that produces an emission spectrum for a whole range of excitation wavelengths. This results in the three-dimensional plot shown. In this case, each of these two plots is for a particular fraction in a chromatographic elution. Thus this instrument is capable of filling a 4-dimensional data matrix.

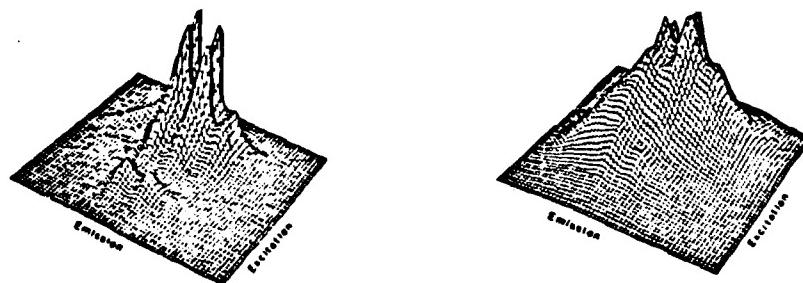


Fig. 4

Another example of a multidimensional instrument is the array detector stopped-flow spectrometer. The array detector is used to obtain the complete absorption spectrum at successive times in the reaction time after the mixing. This allows the changes in the reactant, product, and intermediate concentrations to be followed simultaneously. Additional dimension beyond the three of absorbance, wavelength, and time could be obtained by repetitive experiments while varying temperature, reactant concentration, or chromatographic elution time.

A 3-dimensional instrument in which two dimensions are mass is the recently developed triple quadrupole mass spectrometer shown in Fig. 5 (5). In this instrument, ions from

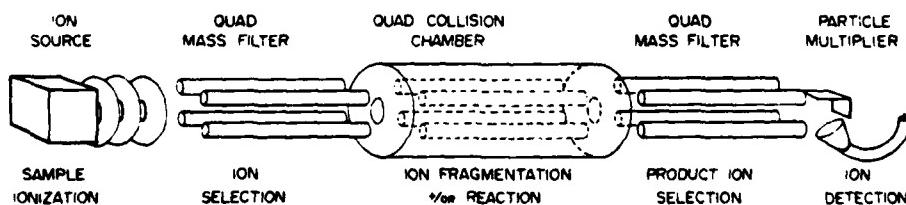


Fig. 5

the source are mass-selected by the first quadrupole and then undergo an ion-molecule reaction with neutral molecules in the center quadrupole collision chamber. The mass spectrum of the ionic products of this reaction (usually simple fragmentation) is then obtained by scanning the mass selected by quadrupole three. The resulting 3-dimensional information array is shown in Fig. 6 (6). The amount of information in the ordinary mass spectrum of this compound, isopropanol, is only the peaks along the foreground diagonal line. The three dimensions of parent mass, daughter mass, and ion intensity are the

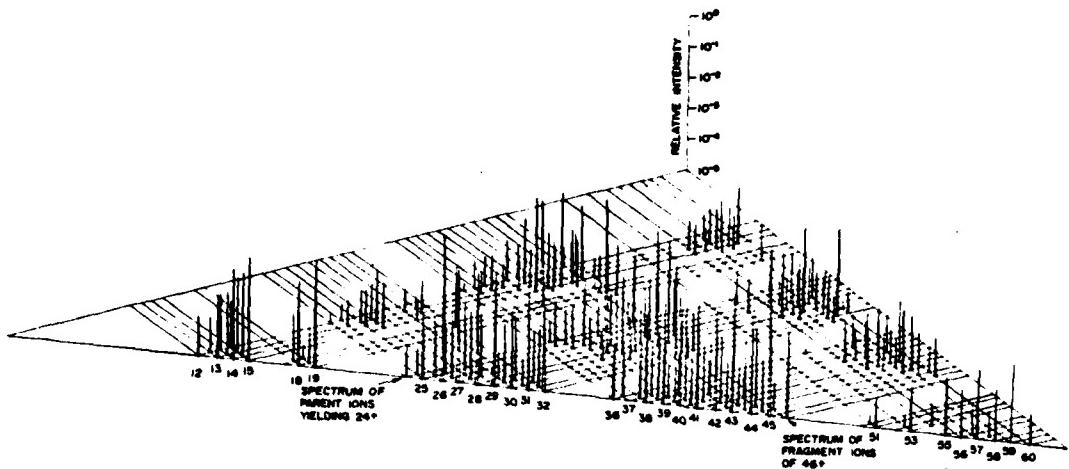


Fig. 6

major ones. We are still investigating additional available dimensions of information. Ones we have found useful so far are electron energy in the source, kinetic energy of the parent ion, and the collision gas pressure. To these must be added the possibility of preselection by chromatography or selective volatilization and selective chemistry in the ionization source and/or collision chamber.

It is clear that these multi-dimensional instruments are capable of producing huge amounts of information about every sample analyzed. It is certainly reasonable to ask how we are going to handle all that data or how we are going to select the most significant data from among all that is possible. Here I will propose two models. The first, shown in Table 2, is the predominant technique currently.

TABLE 2. Post-collection analysis

User	Input sample
Intel. Inst.	Fill n-dimensional data matrix ¹
U/I	Transfer to large batch computer
User	Input analysis options
Comp	Perform analysis ²
Comp	Present results
User	Review results
User	Revise analysis options

- 1. Limited by instrument data rate
- 2. Limited by size of matrix and complexity of analysis

The user loads the sample and an intelligent instrument scans through some number of dimensions to produce the data. This data matrix is then sent to a time-shared batch computer for analysis. Since all the data has been collected before analysis, a variety of analysis methods can be tried to determine the most effective approach. The principal limitations are the time required to collect all the data and the time and computer power necessary to perform a complex analysis on a large data matrix.

TABLE 3. Real-time experimental control

User	Input sample
User	Input analysis goals
RTII	Follow minimized path through all possible data to the most definitive solution(s)*
RTII	Present results and rationale
User	Review results
User	Revise analysis goals

*Limited by the speed of:

Analysis of test results,
Decision on next test,
Instrument response.

The second model, shown in Table 3, motivated our development of triple quadrupole mass spectrometry, but is yet to be implemented in any context as far as I know. This model is like the old general scheme for qualitative inorganic analysis, for those of us old enough or classical enough to remember it. The instrument treats the n-dimensional data matrix as potential data but does not pursue it unless it is relevant to the desired analysis goal(s). This model is based on the fact that one usually doesn't want to know *everything* about a sample. If the sample is complex and the technique is very selective and sensitive, the report could be very lengthy. The fraction of the total possible data that contributes to the result of interest is probably very small. Ideally, then, the analysis time could be reduced by this same factor over the first model. The procedure followed to take only relevant data is to begin by performing some tests for the relevant classes of compounds or phenomena. Only the positive results are followed up with increasingly selective tests that terminate as soon as positive identification and/or accurate quantitation is made. If the original goal statement leads to unsatisfying results, the experiment must be repeated. This model uses the real-time decision-making capability of the computer to the fullest in order to keep high throughput without sacrificing the selectivity available in multidimensional instruments. It requires that the instrument be fractable to computer control and that the interpretation times of the test results are short. In the next section, I will discuss some ways the required computer power might be achieved.

NEW DIRECTIONS IN PROCESSING POWER

It was a major step when the computer entered the laboratory as opposed to the laboratory data being carried to the computer. The concept of the "central" computer has remained, however, even in the laboratory. Thus when additional instruments were computerized, they were often connected to the same minicomputer which was then upgraded to handle multi-tasking and time shared operations. This was viable when the only task for the computer was to automate the data collection from relatively slow instruments. Today, the list of desired computer functions is much longer and a dedicated processor is required. This would not have been economically feasible if it were not for the advent of the microprocessor. However, we are naturally reluctant to give up the now-powerful data processing, display, storage, and programming capability of the well-developed minicomputer. Of course a microprocessor can also be expanded to this capability, but then it is, in cost and fact, the same as a minicomputer. Some of the best of both worlds can be achieved if the dedicated microprocessor remains minimized and is connected along with others to the time-shared minicomputer. This larger computer can provide and share the expensive functions of printing, plotting, storage, and high-level processing while the dedicated microprocessor tends the immediate needs of its instrument. Thus are built the first two levels in a hierarchical system of distributed processing.

The microprocessor part of the instrument can be configured either as a microcomputer or as a process controller. Generally, in the analytical environment, the microcomputer format is preferred for its ability to be reprogrammed and reconfigured as the project evolves and because the division of tasks between the microprocessor and the minicomputer is more flexible. Even so, the microprocessor can be a quite restricting environment. In a programmed integration time linear diode array detector just completed in our lab, the microprocessor was not fast enough for either the data collection (2 MHz) or the integration time control (to the nearest microsecond) so programmable hardware controllers were constructed for those tasks. The microprocessor was then freed for the tasks of data storage, spectrum display, interaction with the operator and the set-up of the acquisition system.

Microprocessors are now frequently used in "smart" devices that are intended to be connected to general-purpose computers. These are subsystems of varying intelligence for which the microprocessor was a convenient building block. Examples of these include terminals, printers, plotters, disk drives, graphics displays, modems, and data loggers. It is no accident that these are all computer peripherals and not analytical instruments. Instrument manufacturers have tended to think of instruments as stand-alone devices rather than elements in an extended information system. The development of standards for data communication between devices is encouraging the inclusion of communication ports in recent instruments.

Several years ago, we were struck with the inherent incompatibility of trying to implement increasingly intelligent control of increasingly complex instrumentation with a microprocessor considerably less powerful than our DEC PDP 11/40 minicomputer. In fact, even the minicomputer could be inadequate for all the high-speed and often simultaneous tasks we projected for an instrument like the triple quadrupole mass spectrometer. Then we realized that with microprocessors under \$25 each, it really wasn't necessary to assign all the tasks to a single processor. Thus we began to design a multiprocessor system for instrumentation applications. This would allow increased power through parallel execution. Recognizing that the timing of simultaneously occurring tasks could all be critical, a major design criterion was that no task execution could interfere with any other. Arranging for the necessary coordination of the task-oriented processors and the exchange of data between them without so much as a hiccup of delay is a problem not addressed by any of the current commercial multiprocessor systems.

We have actually implemented three modes of interprocessor communication. One allows the status of the hardware and program execution of each processor to be continuously available to all the others. Another allows a coordinator processor to load a list of task assignments and execution conditions into any processor without interruption. The third provides for mass transfer of data or programs between a communicator processor and any other. This last one must be performed between time-critical tasks. We believe that parallel processing is desirable for many of the intelligent instruments in the near future and probably essential for the implementation of intelligent real-time experimental control in multi-dimensional instrumentation. Some of the advantages we foresee are listed in Table 4.

TABLE 4. Advantages of parallel processing

Faster Execution

- Parallel execution
- Less time spent in "overhead"
- Simpler addition of hardware controllers and processors

Independent Task Execution

- Non-interference of tasks
- Elimination of task interleaving programs
- Elimination of priority assignment programs
- Simpler task program modification

Modularity of Hardware and Software

- Consolidation of related tasks
- Simpler extension of instrument capability
- Simpler debugging and troubleshooting

As I shall show, the simplification of task coordination software afforded by parallel execution could be a major factor.

THE SOFTWARE BOTTLENECK

The cost of computing hardware continues to plunge while the computing power and ease of interfacing increases. This has made it increasingly easy to put together the hardware to perform complex operations under computer control. The ease of programming complex operations or worse yet, varying combinations of complex operations, has not made similar strides. Thus, as our expectations for the software increase and the hardware costs decrease, software is rapidly becoming the major expense and the limiting factor in the advancement of microcomputer implementation (7). (See Fig. 7.) This will be especially true for scientific instrumentation which lacks the economic base of the word processor or arcade game markets.

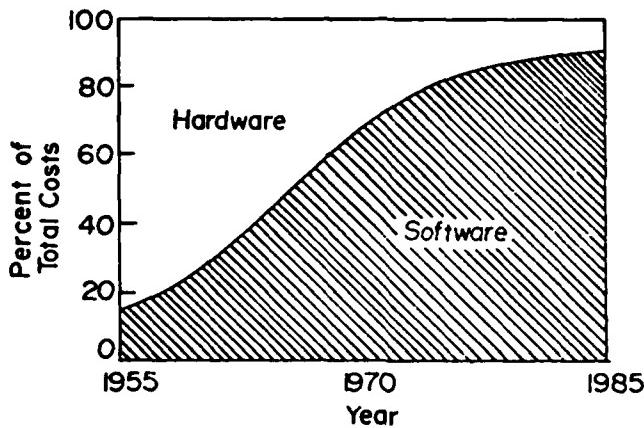


Fig. 7

This condition will not be cured by hiring more programmers; fundamental breakthroughs are required. These could come in either of two areas, both of which invoke the computer to aid in solving its own problem. One of the areas of effort is in the development of a program which can write programs. This would not be just a new language in the sense we know them because the instructions would be to the program writer, not to the computer. Therefore, it will not be a higher-level computer language (which would tend to be more specific to particular types of tasks) but a meta-language that will be more universal. Such a program will not be run with our microcomputers, but we will use it on large computers to generate programs written in a language which microcomputers can compile. Another area of effort is in the development of microcomputers that execute high-level programs directly (8). Two microprocessors are already available from Intel and Zilog that directly execute programs written in an abridged BASIC. Such processors will speed execution, simplify programming, and further reduce hardware requirements.

TOMORROW'S INSTRUMENTALISTS

I have explored in this talk what are possible--even likely trends and capabilities for intelligent instruments in the future. Now, if we want to have such instruments available to advance our science and to apply them in the social fields of energy, health, and environment, how are we going to bring them about? Who is going to explore these new directions so that a few years from now we can see them displayed at the Pittsburgh Conference? Just as fundamental work in solid-state physics spawned the great semiconductor revolution, science often explores and explains new phenomena which the technological side of society then reduces to practice. This process is not strictly linear, however, because this same technology supplies the tools that are necessary for the next advances in science. We must recognize that the technology side of this cycle is driven by the economy, not by scientific altruism or curiosity. That is why the sophistication in the computer-based office equipment and entertainment devices is far beyond that in our latest instrumentation. It is somewhat sobering to realize, in fact, that we would not have microprocessors to use in our instruments at all, if it were not for the military, business, and entertainment markets. In order to keep the cycle going, scientists must be involved in the feedback from technology as well as the feed forward.

This function has not generally been recognized by scientists as essential. A recent analysis, summarized in Table 5 shows that many significant scientific advances that have impacted scientific instrumentation have done so ten-to-twenty years after their first commercial use. I believe it is in our best interests to shorten this cycle significantly.

TABLE 5. Typical areas of technological impact*

Field	Theory	Inventions	Use	Instruments
Communications	1860-1900	1880-1920	1920-1940	1940-1950
Distance Measure	1900	1940	1945-1955	1950-1960
Drugs	1900	1930-1940	1940-1950	1960-1970
Control Systems	1930	1930-1940	1950-1970	1960-1980
Computation	1940	1940-1960	1950-1970	1970-1980

*From Charles H. House, "Perspectives on Dedicated and Control Processing," Computer, Dec. 1980, pp. 35-49.

This could be aided greatly by making sure that our students have available the opportunity for formal education in the principles of electronics, computer science and statistical analysis. I join Bruce Kowalski in his call for the recognition of the subdiscipline of Information Science as an integral part of the science of chemistry. Whether the practitioners of this field are chemometrists or instrumentalists, they will combine solid chemistry with the principles of electronic and computational data manipulation to develop the bases for the tools we need for the future. After all, if we are going to put intelligence in chemical instruments, it should be the chemists' intelligence we put there.

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